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# ME469: Review: Discretization, low-Mach, splitting/stabilization, advection stabilization

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SAND2018-4536 PE

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# Fundamentals of Discretization: Surface vs Volume Integrations

- Given a partial differential equation (PDE) and associated volumetric form:

$$\int \frac{\partial F_j}{\partial x_j} dV = \int S dV$$

- Applying Gauss Divergence provides the standard finite volume form for fluxes in surface integral form (no distinction between internal control volume faces and boundary faces):

$$\sum_k \int_{\Omega_k} \frac{\partial F_j}{\partial x_j} d\Omega_k = \sum_k \int_{\Omega_k} S d\Omega_k \longrightarrow \sum_k \int_{\Gamma_k} F_j n_j d\Gamma_k = \sum_k \int_{\Omega_k} S d\Omega \longrightarrow \int F_j n_j dS = \int S dV$$

- We can also multiple PDE by an arbitrary test function, w, and integrate over a volume,

$$\int w \frac{\partial F_j}{\partial x_j} dV = \int w S dV$$

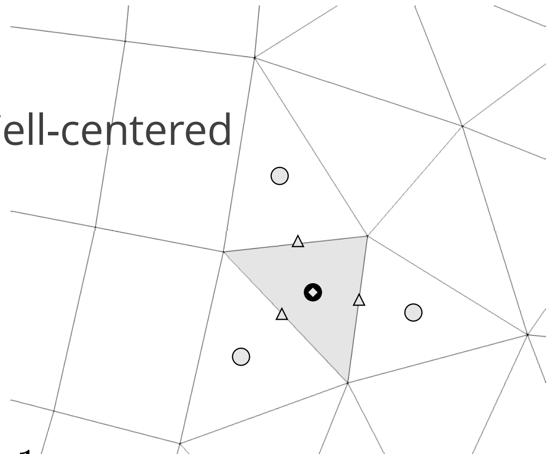
Next, integrate by parts and apply Gauss-Divergence. Note, that test function must be differentiable – shown here, at least once..

$$-\int F_j \frac{\partial w}{\partial x_j} dV + \int \frac{\partial w F_j}{\partial x_j} dV = \underbrace{-\int F_j \frac{\partial w}{\partial x_j} dV}_{\text{Interior}} + \underbrace{\int w F_j n_j dS}_{\text{Boundary}}$$

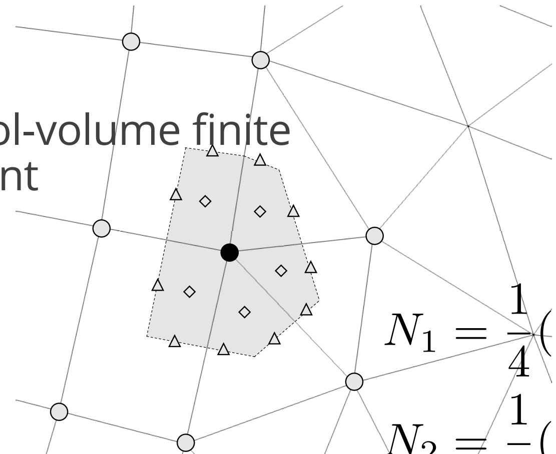
$$\frac{\partial w F_j}{\partial x_j} = w \frac{\partial F_j}{\partial x_j} + \frac{\partial w}{\partial x_j} F_j$$

# Discretization Approaches: Two-state (Left) and Element-based (right)

- Cell-centered



- Control-volume finite element



$$N_1 = N_2 = \frac{1}{2}$$

$$\phi_{ip} = \sum_n N_n^{ip} \phi_n$$

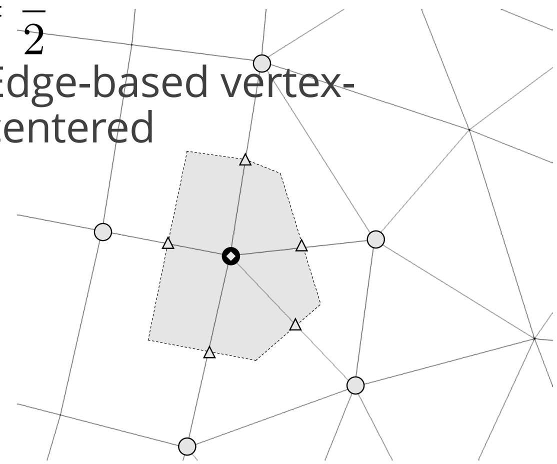
$$N_1 = \frac{1}{4}(1-\xi)(1-\eta)$$

$$N_2 = \frac{1}{4}(1+\xi)(1-\eta)$$

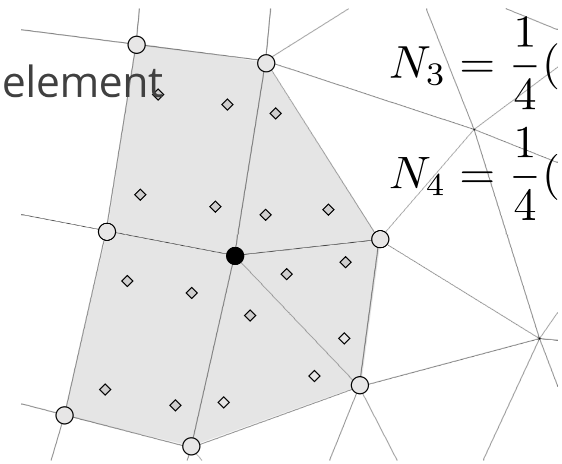
$$N_3 = \frac{1}{4}(1+\xi)(1+\eta)$$

$$N_4 = \frac{1}{4}(1-\xi)(1+\eta)$$

- Edge-based vertex-centered



- Finite element



# Final low-Mach Equation Set

The resulting Equation set is as follows:

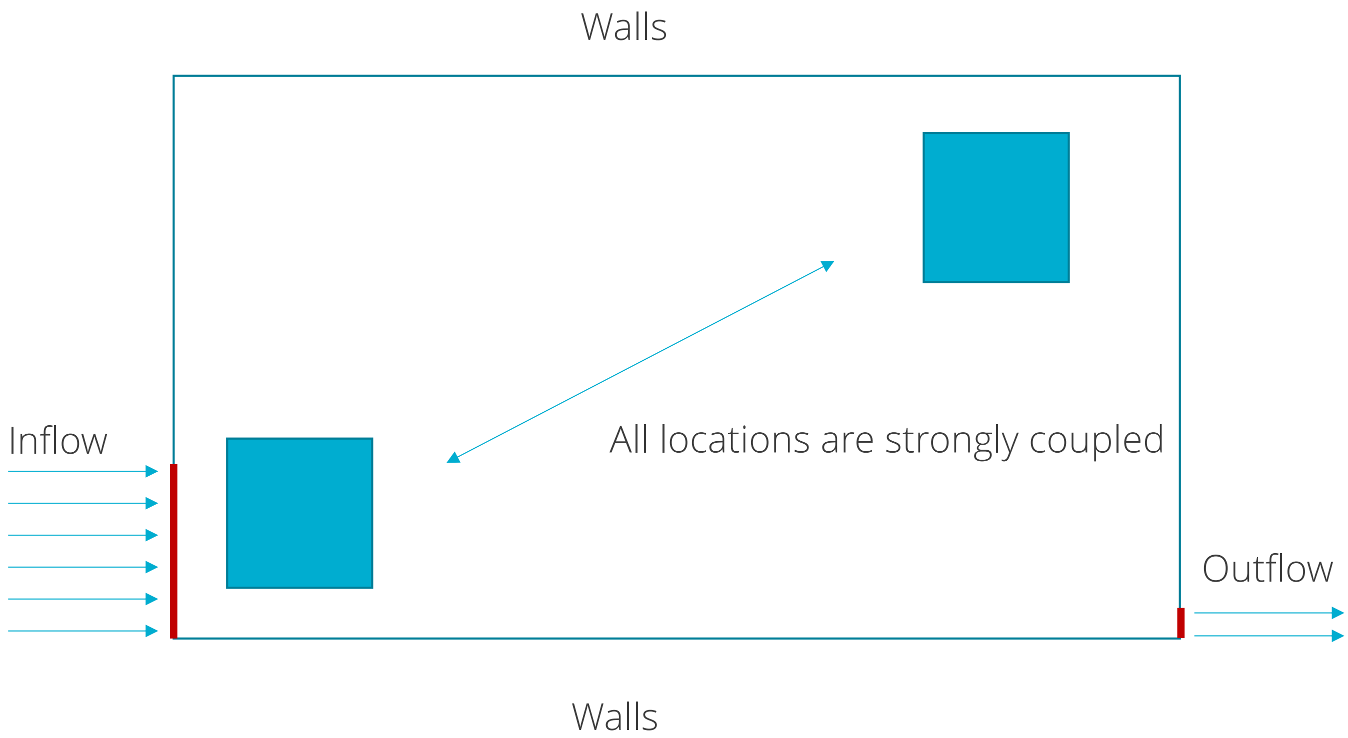
$$\left.\begin{aligned}
&\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0, \\
&\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_j} + \frac{\partial p^m}{\partial x_i} = \frac{\partial \tau_{ij}}{\partial x_j} + (\rho - \rho_\circ)\, g_i, \\
&\frac{\partial \rho h}{\partial t} + \frac{\partial \rho u_j h}{\partial x_j} = -\frac{\partial q_j}{\partial x_j} + \frac{\partial P_{th}}{\partial t}
\end{aligned}\right\} \underline{\text{2+nDim}}$$

- Equation of state given by the thermodynamic pressure: $\rho = \frac{P_{th} M}{RT}$
- Energy transport is only required when the system modeled has a temperature difference

<u>EOS does not provide an equation for closure</u>: An alternative approach is required for motion pressure!

# Thought Experiment… Solver Ramifications

- For Elliptic systems, fixed point iterative solvers fail since the sequential propagation of information is not adequate for a system with infinite wave speeds



# Multigrid Methods: The Approach

- Multigrid methods (MG) are essential for efficient solver performance in fluids-based Elliptic systems
- In simple, structured domains, this can be geometric (GMG), while in unstructured, algebraic (AMG)

$$A\phi = f$$

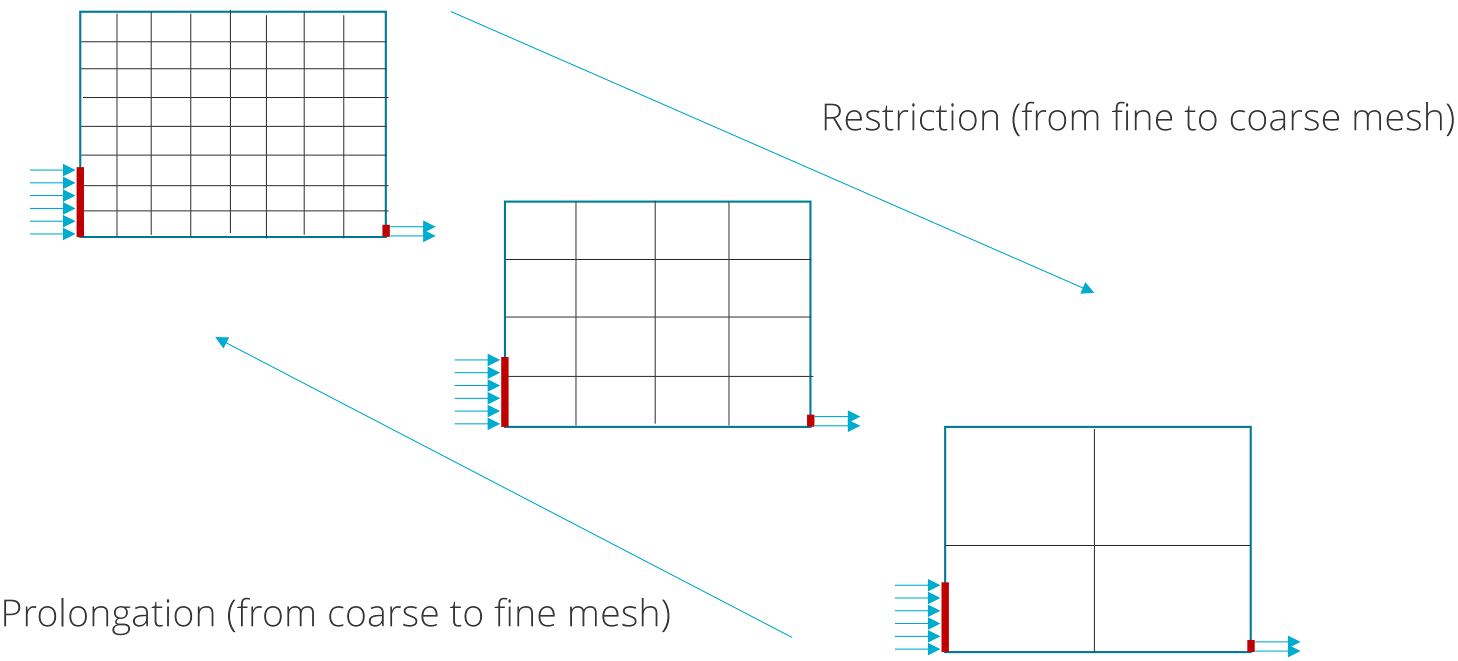
$$\epsilon = \phi - \tilde{\phi}$$

$$r = f - A\tilde{\phi}$$

$$A\left(\tilde{\phi} + \epsilon\right) = f$$

$$A\epsilon = r$$

$$\phi = \tilde{\phi} + \epsilon$$



# Multigrid Methods: V- and W-Cycles

Briggs (2000)

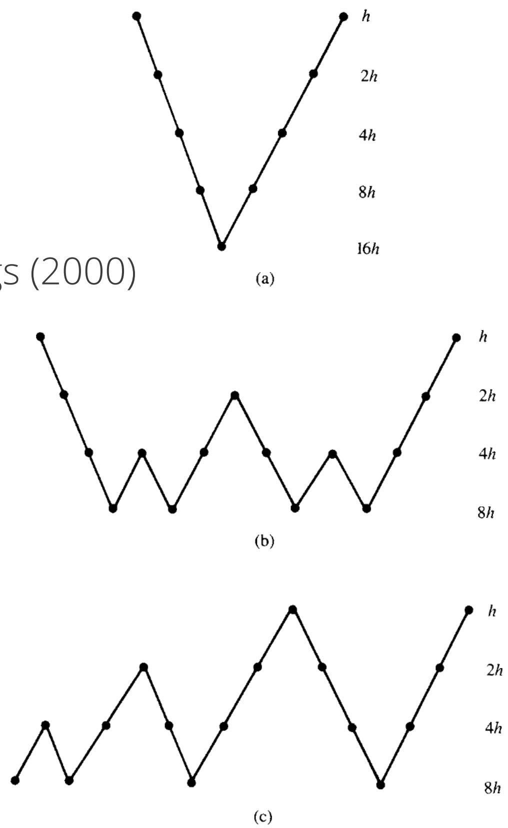
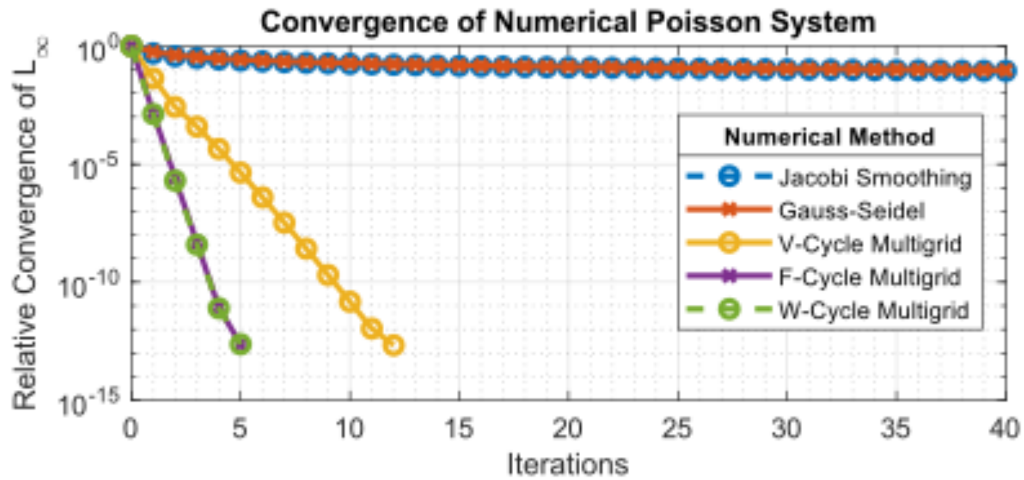



Figure 3.6: *Schedule of grids for* (a) *V-cycle,* (b) *W-cycle, and* (c) *FMG scheme, all on four levels.*




https://en.wikipedia.org/wiki/Multigrid_method

# Pressure Projection and Block Factorization

- Semi-discrete approach (uniform density)

$$\rho \frac{\hat{u}_i - u_i^n}{\Delta t} + \frac{\partial}{\partial x_j}\left(\rho \hat{u}_i u_j^n\right) = -\frac{\partial p^n}{\partial x_i} + \frac{\partial \hat{\tau}_{ij}}{\partial x_j}$$

$$\rho \frac{u_i^{n+1} - \hat{u}_i}{\Delta t} = -\frac{\partial}{\partial x_i}\left(p^{n+1} - p^n\right)$$

$$\frac{\partial^2}{\partial x_i^2}\left(p^{n+1} - p^n\right) = \frac{\rho}{\Delta t}\frac{\partial \hat{u}_i}{\partial x_i}$$

  - Chorin (1968)
  - Time scale is the time step:

$$u_i^{n+1} = \hat{u}_i - \Delta t\left(\tfrac{1}{\rho}\tfrac{\partial}{\partial x_i}\left(p^{n+1} - p^n\right)\right)$$

- Fully discrete approach

$$\begin{bmatrix} \mathbf{A} & \mathbf{G} \\ \mathbf{D} & \mathbf{0} \end{bmatrix} \begin{Bmatrix} \mathbf{U}^{n+1} \\ \mathbf{P}^{n+1} \end{Bmatrix} = \begin{Bmatrix} \mathbf{f} \\ \mathbf{0} \end{Bmatrix}$$

  - Factored matrix:

$$\begin{bmatrix} \mathbf{A} & \mathbf{G} \\ \mathbf{D} & \mathbf{0} \end{bmatrix} \approx \begin{bmatrix} \mathbf{A} & \mathbf{0} \\ \mathbf{D} & -\mathbf{D}\bar{\mathbf{A}}^{-1}\mathbf{G} \end{bmatrix} \begin{bmatrix} \mathbf{I} & \bar{\mathbf{A}}^{-1}\mathbf{G} \\ \mathbf{0} & \mathbf{I} \end{bmatrix}$$

  $\bar{\mathbf{A}}^{-1}$ is an approximation to $\mathbf{A}^{-1}$

  - SIMPLE family of methods
  - Time scale is the characteristic scale of $\bar{\mathbf{A}}^{-1}$:

$$\mathbf{U}^{n+1} = \hat{\mathbf{U}} - \bar{\mathbf{A}}^{-1}\mathbf{G}\mathbf{P}^{n+1}$$

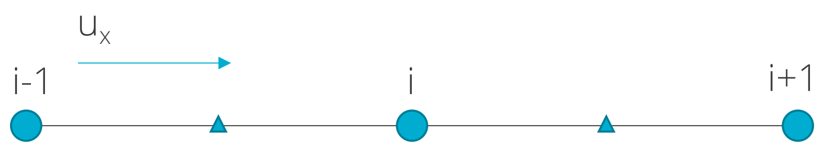
    - For convection-dominated flows, this looks like Δx/U

$$\begin{bmatrix} \boldsymbol{A} & \boldsymbol{G} \\ \boldsymbol{D} & 0 \end{bmatrix} \begin{bmatrix} u^{n+1} \\ p^{n+1} \end{bmatrix} = \begin{bmatrix} \boldsymbol{f} \\ 0 \end{bmatrix} + \begin{bmatrix} (\boldsymbol{I} - \boldsymbol{A}\tau)\boldsymbol{G}(p^{n+1} - p^n) \\ \tau(\boldsymbol{L} - \boldsymbol{D}\boldsymbol{G})(p^{n+1} - p^n) \end{bmatrix}$$

## Monotonic Issues at High Pe: Simple Matrix Analysis

Consider our passive scalar concentration whose natural range (as a mass fraction) is bounded between zero and unity, here, shown as a stationary transport equation:

$$\frac{\partial \rho u_j \phi}{\partial x_j} - \frac{\partial}{\partial x_j}\left(\rho D \frac{\partial \phi}{\partial x_j}\right) = 0$$




Using our CDS and standard diffusion operator yields the following matrix system:

$$\left(\frac{\rho u}{2}\begin{bmatrix}-1 & 0 & 1\end{bmatrix} + \frac{\rho D}{\Delta x}\begin{bmatrix}-1 & 2 & -1\end{bmatrix}\right)\begin{bmatrix}\phi_{i-1}\\ \phi_i \\ \phi_{i+1}\end{bmatrix}.$$

$$a_{i,i-1} = \frac{\rho D}{\Delta x}\left(1 + \frac{Pe}{2}\right)$$

With coefficients, $a_{i,i}\phi_i = a_{i,i-1}\phi_{i-1} + a_{i,i+1}\phi_{i+1}$ and: $a_{i,i} = (a_{i,i-1} + a_{i,i+1})$

$$a_{i,i+1} = \frac{\rho D}{\Delta x}\left(1 - \frac{Pe}{2}\right)$$

Positive for Pe < 2

Substituting: $a_{i,i-1} = a_{i,i} - a_{i,i+1}$ and defining: $\xi = \frac{a_{i,i+1}}{a_{i,i}}$

Yields: $\phi_i = \xi\phi_{i+1} + (1-\xi)\phi_{i-1}$

For Pe < 2, the value of the scalar at node i is <u>a linear combination of the neighboring values</u>

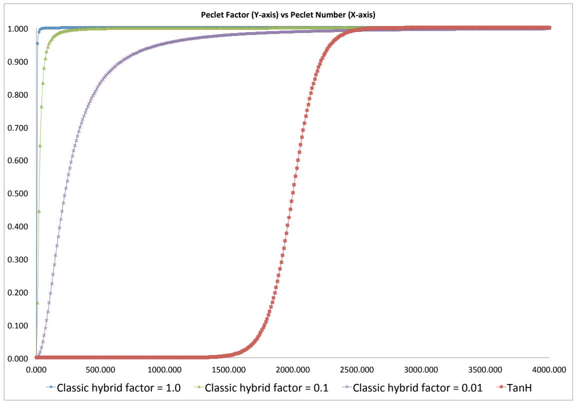
# Monotonic Issues at high Pe: Alternative View (Diagonal Dominance)

Define Diagonal Dominance as: $$\frac{\sum_{i \neq j} |a_{i,j}|}{|a_{i,i}|} \leq 1$$

For a monotonic operator and ease of solving the linear system, diagonal dominance is desired

In our advection/diffusion case, this is expressed as:

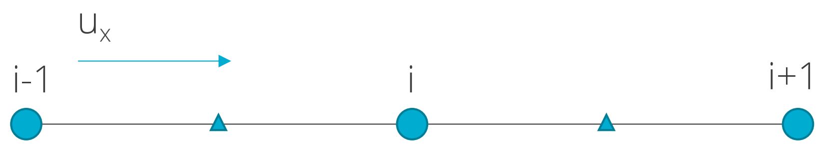
$$\frac{\left|\frac{\rho D}{\Delta x}\left(1 - \frac{Pe}{2}\right)\right| + \left|\frac{\rho D}{\Delta x}\left(1 + \frac{Pe}{2}\right)\right|}{\frac{2\rho D}{\Delta x}} \leq 1$$




Which, again, is only ensured when the Peclet number is less than two

# Monotonic Issues Resolved When Using First-order Upwind

$$\frac{\partial \rho u_j \phi}{\partial x_j} - \frac{\partial}{\partial x_j}\left(\rho D \frac{\partial \phi}{\partial x_j}\right) = 0$$




$$a_{i,i-1} = \frac{\rho D}{\Delta x}(1 + Pe)$$

Positive for all Pe

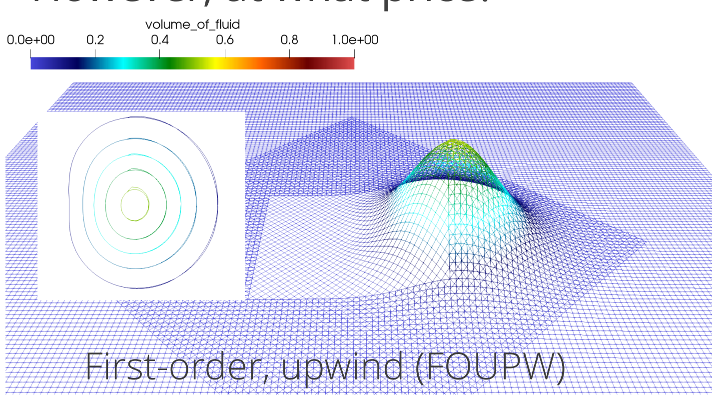
$$a_{i,i} = (a_{i,i-1} + a_{i,i+1})$$

$$a_{i,i+1} = \frac{\rho D}{\Delta x}$$

$$\left(\frac{\rho u}{2}\begin{bmatrix}-1 & 1 & 0\end{bmatrix} + \frac{\rho D}{\Delta x}\begin{bmatrix}-1 & 2 & -1\end{bmatrix}\right)\begin{bmatrix}\phi_{i-1}\\ \phi_i \\ \phi_{i+1}\end{bmatrix}$$

$$\phi_i = \xi \phi_{i+1} + (1-\xi)\phi_{i-1} \qquad \xi = \frac{a_{i,i+1}}{a_{i,i}}$$

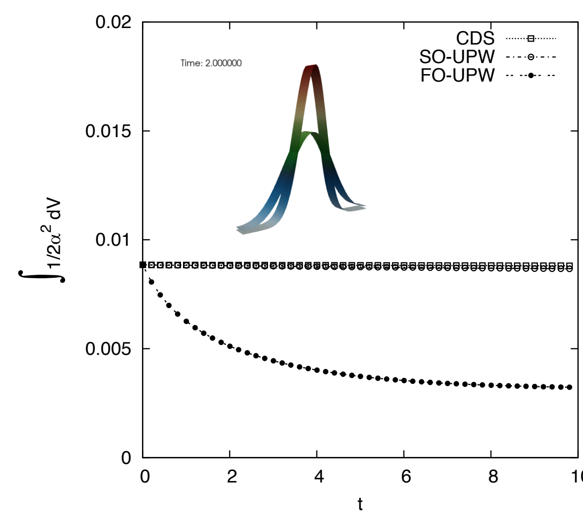
However, at what price?




Volume-of-fluid example (Domino and Horne, Renew. Ener. 2022)

Fully bounded with diagonal dominance

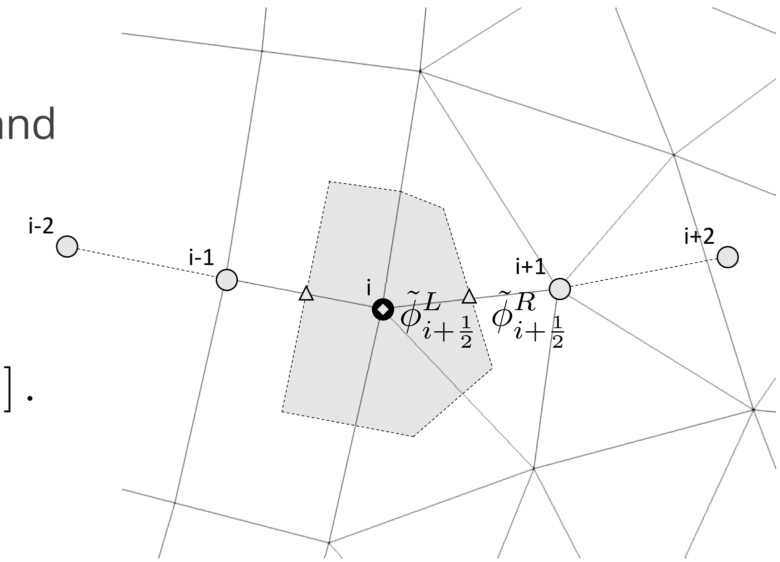
$$\frac{\sum_{i \neq j} |a_{i,j}|}{|a_{i,i}|} \leq 1$$



# General Kappa-Method of Hirsh

## Numerical Computation of Internal and External Flows, vol. 2, John Wiley & Sons, 1990

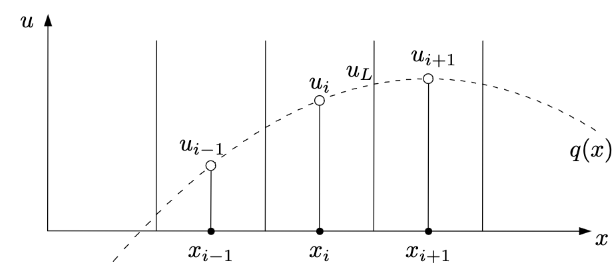
For the edge defined by the i and i+1 node, define a Left and Right state:




$$\tilde{\phi}^L_{i+\frac{1}{2}} = \phi_i + \frac{1}{4}\left[(1-\kappa)\left(\phi_i - \phi_{i-1}\right) + (1+\kappa)\left(\phi_{i+1} - \phi_i\right)\right],$$

$$\tilde{\phi}^R_{i+\frac{1}{2}} = \phi_{i+1} - \frac{1}{4}\left[(1+\kappa)\left(\phi_{i+1} - \phi_i\right) + (1-\kappa)\left(\phi_{i+2} - \phi_{i+1}\right)\right].$$

- For $\kappa$ = +1, we simply revert to CDS
- For $\kappa$ = -1, Second-order upwind
- For $\kappa$ = 2/3, QUICK (Leonard, "A stable and accurate convective modelling procedure based on quadratic up-stream interpolation", Comput. Methods Appl. Mech. Eng. 19 (1979) 59–98.)

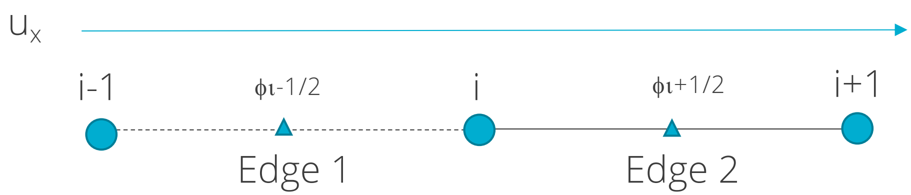



Quadratic basis (three-points required)

## Classic Flux Limiters

**Van Leer, B. (1974), "Towards the ultimate conservative difference scheme II. Monotonicity and conservation combined in a second order scheme", J. Comput. Phys., 14 (4): 361–370**

- Consider our standard three-point stencil obtained by iterating edge 1 and 2




- In the above stencil, we are stressing that when iterating edge 2, we do not have information easily obtain for edge 1 (shown above as a dashed line); (speaking from an unstructured perspective)

$$\phi_{i+\frac{1}{2}} = \phi^{LOW}_{i+\frac{1}{2}} - \Phi(r_{i+\frac{1}{2}}) \left( \phi^{LOW}_{i+\frac{1}{2}} - \phi^{HIGH}_{i+\frac{1}{2}} \right)$$

Monotonic upstream-centered scheme for conservation laws (MUSCL)

- Above, the “LOW” and ”HIGH” are any operators that you select, e.g.,

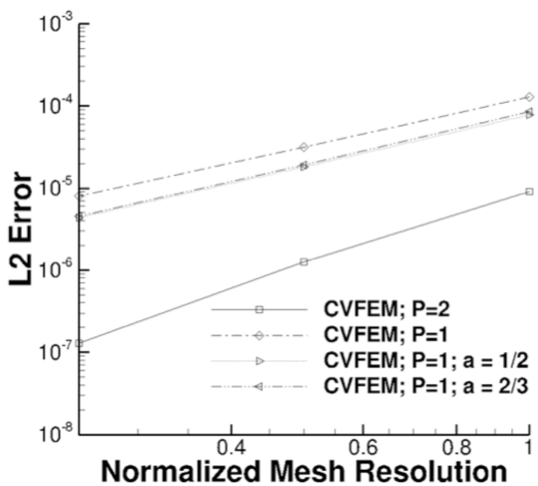
$$\phi^{LOW}_{i+\frac{1}{2}} = \phi_i \qquad \phi^{HIGH}_{i+\frac{1}{2}} = \frac{\phi_i + \phi_{i+1}}{2} \longrightarrow \phi_{i+\frac{1}{2}} = \phi_i + \frac{1}{2}\Phi(r_{i+\frac{1}{2}})\left(\phi_{i+1} - \phi_i\right)$$

$$r_{i+\frac{1}{2}} = \frac{(\phi_i - \phi_{i-1})}{(\phi_{i+1} - \phi_i)} \qquad (\phi_i - \phi_{i-1}) = 2G_x\phi_i\Delta x - (\phi_{i+1} - \phi_i) \qquad G_x\phi_i = \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x}$$

# Blending Approaches to Arrive at Pseudo Higher-order Methods: Upwind and Central

Define an upwind operator now at an arbitrary integration point:

$$\phi_{ip}^{UPW} = \alpha_{upw}\tilde{\phi}_{ip}^{L} + (1-\alpha_{upw})\,\phi_{ip}^{CDS};\, \dot{m} > 0,$$
$$\alpha_{upw}\tilde{\phi}_{ip}^{R} + (1-\alpha_{upw})\,\phi_{ip}^{CDS};\, \dot{m} < 0.$$




And for a generalized CDS scheme:

$$\phi_{ip}^{GCDS} = \frac{1}{2}\left(\hat{\phi}_{ip}^{L} + \hat{\phi}_{ip}^{R}\right), \qquad \hat{\phi}_{ip}^{L} = \alpha\tilde{\phi}_{ip}^{L} + (1-\alpha)\,\phi_{ip}^{CDS}, \quad \hat{\phi}_{ip}^{R} = \alpha\tilde{\phi}_{ip}^{R} + (1-\alpha)\,\phi_{ip}^{CDS}$$

- Two new blending parameters: $\alpha_{upw}$ and $\alpha$